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ROHM AND HAAS COMPANY

August 1, 2006

Mr. Stephen L. Johnson, Administrator
US Environmental Protection Agency
P.O. Box 1473
Merrifield, VA 22116

Attn.: Chemical Right-to-Know Program

RE: HPV CHEMICAL CHALLENGE PROGRAM for
2-Pentanamine, 2,4,4-trimethyl (Primene™ TOA; CAS No. 107-45-9)
Rohm and Haas Chemicals, LLC

Dear Mr. Johnson,

Rohm and Haas Chemicals, LLC is pleased to submit the test plan and robust summaries for 2-Pentanamine, 2,4,4-trimethyl (Primene™ TOA; CAS No. 107-45-9). The company has agreed to sponsor this chemical and provide the Agency with the enclosed information in the year 2006.

We have electronically submitted via e-mail, the test plan (.doc and .pdf) and IUCLID robust summaries (.rtf and .pdf), as well as this cover memo.

We understand this information will be posted on the internet for comments for a period of 120 days. Please forward comments to me at the address below.

Regards,

James E. McLaughlin, Ph. D.
Program Manager
Toxicology Department
Rohm and Haas Chemicals, LLC
727 Norristown Road
P.O. Box 0904
Spring House, PA 19477-0904
Phone: 215-641-7459

HIGH PRODUCTION VOLUME (HPV) CHALLENGE PROGRAM

Test Plan for 2-Pentanamine, 2,4,4-trimethyl- (Primene™ TOA) CAS Number 107-45-9

Prepared By:

Rohm and Haas Chemicals, LLC

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OVERVIEW

The Rohm and Haas Chemicals, LLC hereby submits for review and public comment the test plan for 2-Pentanamine, 2,4,4-trimethyl- (Primene™ TOA) (CAS Number 107-45-9) under the Environmental Protection Agency's (EPA) High Production Volume (HPV) Chemical Challenge Program. Here we provide existing data on 2-Pentanamine, 2,4,4-trimethyl-, and list additional testing to be performed to adequately fulfill the Screening Information Data Set (SIDS) for physico-chemical, environmental fate, ecotoxicity and human health effects endpoints.

2-Pentanamine, 2,4,4-trimethyl- (Primene™ TOA) is a strong base, C_8 primary amine in which the nitrogen atom is linked to a tertiary carbon atom. Primene™ TOA is used primarily as an intermediate for making salts and derivatives. Many applications of Primene™ TOA result from its unique physical and chemical properties which differ markedly from those of related straight-chain or less branched isomers. It is a mobile liquid at ambient temperature and maintains its low viscosity down to very low temperatures. Primene™ TOA is much more soluble in petroleum solvents than analogous less branched amines. These advantageous properties are thought to arise from its highly branched structure and a low tendency toward crystallization. In addition, it shows outstanding color stability because of its high resistance to oxidation.

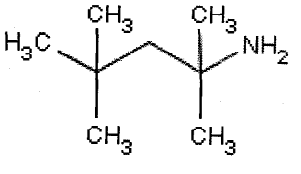
New and additional testing is required to fulfill the SIDS endpoints. A testing program has been designed with the intention of satisfying these requirements.

GENERAL INFORMATION

CAS Number: 107-45-9

Molecular Weight: 129

Structure and Formula: $C_8H_{19}N$



TEST PLAN SUMMARY

CAS No. 107-45-9	Information	OECD Study	Estimation	GLP	Acceptable	New Testing Required
Study	Y/N	Y/N	Y/N	Y/N	Y/N	Y/N
Physical/Chemical Data						
Melting Point	N	-	-	-		Y
Boiling Point	N	-	-	-	-	Y
Density	Y	N	-	N	Y	N
Vapor Pressure	N	-	-	-	-	Y
Partition Coefficient	Y	N	-	N	Y	N
Water Solubility	N	-	-	-	-	Y
Dissociation Constant (pH and pKa Values)	Y	N	-	N	Y	N
Other P/C Studies						
Flash Point	Y	N	-	N	Y	-
Pour Point	Y	N	-	N	Y	-
Surface Tension/Interfacial Tension with Water	Y	N	-	N	Y	-
Environmental Fate and Pathway						
Photodegradation	Y	-	Y	-	Y	N
Stability in Water (Hydrolysis)	Y	-	-	-	-	N
Transport and Distribution (Fugacity)	Y	-	Y	-	Y	N
Biodegradation	N	-	-	-	-	Y
Ecotoxicity						
Acute Toxicity to Fish	N	-	-	-	-	Y
Acute Toxicity to Daphnia	N	-	-	-	-	Y
Toxicity to Algae	N	-	-	-	-	Y
Toxicity						
Acute Oral	Y	Y	-	Y	Y	N
Repeated Dose	N	-	-	-	-	Y
Genetic Toxicity in vitro						
Gene Mutation	Y	Y	-	Y	Y	N
Genetic Toxicity in vivo	N	-	-	-	-	Y
Reproduction Toxicity	N	-	-	-	-	Y
Development/Teratogenicity	N	-	-	-	-	Y
Human Experience	N	-	-	-	-	-
Other Toxicity Studies						
Skin Irritation	Y	Y	-	Y	Y	-
Eye Irritation	Y	-	-	-	Y	-

TEST PLAN DESCRIPTION FOR EACH SIDS ENDPOINT

A. Physicochemical

Melting Point- This endpoint will be tested using OECD 102 to fill the SIDS requirement.

Boiling Point- This endpoint will be tested using OECD 103 to fill the SIDS requirement.

Density- A value for this endpoint was determined using an Anton-Paar DMA-46 densitometer at the Analytical Research Department of the Rohm and Haas Company in Spring House, PA. No data on whether the test was conducted in compliance with GLP, but was reviewed internally and has been deemed valid.

Vapor Pressure- This endpoint will be tested using OECD 104 to fill the SIDS requirement.

Partition Coefficient- A value for this endpoint was determined from analyses that followed the Shake Flask Method. This test was not conducted in compliance with GLP, but was reviewed internally and has been deemed valid.

Water Solubility- This endpoint will be tested using OECD 105 to fill the SIDS requirement.

Dissociation Constant- A value for this endpoint was determined by Potentiometric titration to measure the Half Neutralization Potential (HNP). From this result a pKa value was estimated. This test was not conducted in compliance with GLP, but was reviewed internally and has been deemed valid.

Conclusion- Testing will be conducted to satisfy those SIDS endpoints which have not been filled.

B. Environmental Fate and Pathway

Photodegradation- This endpoint is satisfied by estimation.

Stability in Water- It was attempted to satisfy this endpoint by estimation.

Transport and Distribution- This endpoint is satisfied by estimation.

Biodegradation- This endpoint will be tested using OECD 301B to fill the SIDS requirement.

Conclusion- No data for these endpoints exists. Modeling/estimation was conducted to satisfy the photodegradation, hydrolysis and fugacity endpoints. Testing will be conducted to satisfy the biodegradation endpoint.

C. Ecotoxicity Data

Acute Toxicity to Fish- This endpoint will be tested using OECD 203 to fill the SIDS requirement.

Acute Toxicity to Aquatic Invertebrates- This endpoint will be tested using OECD 202 to fill the SIDS requirement.

Acute Toxicity to Aquatic Plants- This endpoint will be tested using OECD 201 to fill the SIDS requirement.

Conclusion- No data for these endpoints exists. Testing will be carried out according to the applicable OECD guidelines.

D. Toxicological Data

Acute Toxicity- This endpoint is filled by data from a study assessing toxicity following oral exposure. Acute oral toxicity was evaluated in male and female rats. In addition, a study was conducted in rabbits to assess skin irritation, and based on the corrosive results of the study a determination was made for eye irritation. The studies were conducted in compliance with GLP. The quality of the study is deemed as reliable without restrictions.

Repeated Dose- This endpoint has not been determined and will be tested using OECD 422 to satisfy the SIDS requirement.

Genetic Toxicity Mutation- This endpoint is filled with data from a study that followed OECD Test Guideline 471 and was conducted under GLP regulations. This study utilized Salmonella typhimurium strains TA98, TA100, TA1535 and TA1537 in the presence and absence of a metabolic activation system. The quality of this study was deemed as reliable without restrictions.

Mouse Micronucleus Assay- This endpoint has not been determined and will be tested using OECD 474 to satisfy the SIDS requirement.

Reproductive Toxicity- This endpoint has not been determined and will be tested using OECD 422 to satisfy the SIDS requirement.

Developmental Toxicity- This endpoint has not been determined and will be tested using OECD 422 to satisfy the SIDS requirement.

Conclusion- Acute toxicity and gene mutation SIDS endpoints have been satisfied from existing studies. Testing will be conducted to satisfy those SIDS endpoints which have not been filled. The Repeat Dose Toxicity, Reproductive/Developmental Toxicity

endpoints will be satisfied by conducting testing using OECD 422. Combining the testing in a single protocol will require the use of fewer animals.

SIDS DATA SUMMARY

Data determining the density was obtained from actual testing using a densitometer. A value of 0.7698 g/cc was measured. Data determining the partition coefficient was obtained from actual testing by the shake flask method. A log P of 1.09 $\pm$ 0.20 was calculated. Data determining the dissociation constant was obtained using Potentiometric titration in non-aqueous solvent to determine the Half Neutralization Potential because the test substance was not sufficiently water soluble. From this, the pK_a value of 10.5 was estimated.

The AOP Model v 1.91 resident within EPIWIN was used to estimate atmospheric degradation of Primene™ TOA. For hydroxyl radical reactions AOPWIN estimated the hydrogen abstraction rate constant to be 2.25E-12 cm^3/molecule-sec. The reaction rate with N, S, and –OH was estimated to be 21.0E-12 cm^3/molecule-sec. The overall OH radical rate constant was estimated to be 23.25E-12 cm^3/molecule-sec. The estimated half-life equaled 5.52 hours assuming a 12 hour day and 1.5E06 OH/cm^3. The model was unable to estimate ozone reaction kinetics because no structurally similar molecules were within the database.

HYDROWIN was unable to estimate hydrolysis rate constant because no similar chemical structures are in the database.

The Level I fugacity model calculates the distribution of a fixed quantity 1.0E05 kg of a conserved, i.e., non-reacting chemical in a closed environment at equilibrium, with no degrading reactions, no advective processes and no intermedia transport. The medium receiving the emission is unimportant because the chemical is assumed to become instantaneously distributed.

The Level III Fugacity model calculates the steady state distribution of a chemical, in an environment not at equilibrium. The chemical is continuously discharged at a constant rate, 1000 kg/hr, into the chosen environmental media, and achieves a steady-state condition at which input and output rates are equal. This involves calculating the rates of degradation and advection, from half-lives or rate constants, and advective flow rates and considering the emission. Intermedia transport processes (e.g. wet deposition, evaporation, or sedimentation) are included. The media receiving the emissions are very important and have a controlling influence on the overall fate of the chemical.

The environmental fate parameters used in determining the fugacity of Primene™ TOA were derived using EPIWIN v 3.12 and include:

Molecular weight: 129.25
Water Solubility: 10670 (mg/L)
Vapor pressure: 8.03 mm Hg, 1070.58 Pa (estimated using MPBPWIN)

Log Kow: 2.58 (estimated using KOWWIN)
Melting Point: -20.02 (estimated using MPBPWIN)
Half-lives (h):
Air: 11
Water: 900
Soil: 1.8E03
Sediment: 8.1E03

The half-lives in the environmental media were generated using the Level III fugacity model resident in EPIWIN employing the estimated environmental fate parameters. The Level III fugacity model resident within EPIWIN is based on the EQC model. The advantage of using the stand alone model is that it can be parameterized to generate Level I, II or III output.

The following table illustrates the percentage of the chemical in the air, water, soil and sediment compartments based on Level I output.

Table 1. Level I EQC Fugacity Model Compartmental Mass Distribution

Compartment	Mass (percent)	Half-life (hr)
Air	66.1	11
Water	25.3	900
Soil	8.50	1.8E03
Sediment	0.189	8.1E03

Level III output are illustrated in the following table:

Table 2. Level III EQC Fugacity Model Compartmental Mass Distribution

Compartment	Mass (percent)
Air	1.02
Water	19.7
Water: Fish	3.74E-04
Soil	79.1
Sediment	0.187

For the Level III fugacity modeling, continuous discharge of 1000 kg/hour into the air, water and soil compartments was assumed. Partitioning into the sediment compartment was driven by adsorption kinetics. The reaction rate kinetics were estimated to decrease in air, water and soil, respectively. The fugacity parallels this relationship where the atmosphere would serve as the primary "sink" for Primene™ TOA followed by the water compartment, sediment and soil. Based on half-lives and environmental fate characteristics Primene™ TOA would be anticipated to compartmentalize predominantly in the soil (79.1% of the entire mass) and aquatic compartments (19.7% of the entire mass), with lesser mass percentages in biota, air and sediments.

Primene^{TM} TOA is considered moderately toxic following acute oral exposure. The oral LD_{50} of male and female rats (combined) was 217.7 mg/kg. Signs of apparent neurotoxicity were observed in rats treated with up to 500 mg/kg by gavage. Data from a skin irritation study in rabbits indicates that Primene^{TM} TOA is corrosive to the skin, and thus the eye.

Results from a mutagenicity study indicate that Primene^{TM} TOA was not mutagenic in an Ames mutagenicity assay using Salmonella typhimurium with or without metabolic activation.

EVALUATION OF DATA FOR QUALITY AND ACCEPTABILITY

The collected data were reviewed for quality and acceptability following the general US EPA guidance and the systematic approach described by Klimisch *et al.* (1997). These methods include consideration of the reliability, relevance and adequacy of the data in evaluating their usefulness for hazard assessment purposes. This scoring system was only applied to human health endpoint studies per EPA recommendation. The codification described by Klimisch *et al.* (1997) specifies four categories of reliability for describing data adequacy. These are:

(1) Reliable without restriction: Includes studies or data complying with Good Laboratory Practice (GLP) procedures, or with valid and/or internationally accepted testing guidelines, or in which the test parameters are documented and comparable to these guidelines.
(2) Reliable with restriction: Includes studies or data in which test parameters are documented but vary slightly from testing guidelines.
(3) Not reliable: Includes studies or data in which there are interferences, or that use non-relevant organisms or exposure routes, or which were carried out using unacceptable methods, or where documentation is insufficient.
(4) Not assignable: Includes studies or data in which insufficient detail is reported to assign a rating, e.g., listed in short abstracts or secondary literature (books, reviews, etc.)

REFERENCES

1. USEPA. (1999). Determining the Adequacy of Existing Data. Guidance for the HPV Challenge Program. Draft dated 02/10/1999.

2. Klimisch, H.J., M. Andreae and U. Tilmann. (1997). A Systemic Approach for Evaluating the Quality of Experimental Toxicological and Ecotoxicological Data. Regul. Toxicol. Pharmacol. 25:1-5.

3. U.S. Environmental Protection Agency (USEPA), Office of Pollution Prevention and Toxics. 1998. Guidance for Meeting the SIDS Requirements: Chemical Right-to-Know Initiative.

4. Carbone, J.P. (2006). Primene^{TM} TOA Amine Quantitative Structure Activity Relationship Modeling. Toxicology Department Memo 06M-020. Rohm and Haas Chemicals, LLC, Philadelphia, PA.

5. Meylan, W.M. and P.H. Howard. 1999a. User's Guide for EPIWIN, EPI suite: EPI-Estimation programs interface for Microsoft Windows. Syracuse Research Corporation, North Syracuse, NY. 33 pp.

I U C L I D

D a t a S e t

Existing Chemical	ID: 107-45-9
CAS No.	107-45-9
EC No.	203-491-1
EINECS Name	1,1,3,3-tetramethylbutylamine
TSCA Name	2-Pentanamine, 2,4,4-trimethyl-
Molecular Formula	C8H19N
Generic name	Primene TOA

Producer Related Part

Company:	Rohm and Haas Company
Creation date:	17-MAY-2006

Substance Related Part

Company:	Rohm and Haas Company
Creation date:	17-MAY-2006

Printing date:	02-AUG-2006
Revision date:	
Date of last Update:	**02-AUG-2006**

Number of Pages: **28**

Chapter (profile):	Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile):	Reliability: without reliability, 1, 2, 3, 4
Flags (profile):	Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE), Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 Applicant and Company Information

Type: cooperating company
Name: Rohm and Haas Company
Contact Person: Wendy W. Bingaman **Date:**
Street: 727 Norristown Road
Town: Spring House, PA
Country: United States
Phone: 215-619-5531
Telefax: 215-619-1657

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

Type: cooperating company
Name: Rohm and Haas Company
Contact Person: Alexis L. Chapman **Date:**
Street: 727 Norristown Road
Town: Spring House, PA
Country: United States
Phone: 215-619-5945
Telefax: 215-619-1618

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.0.2 Location of Production Site, Importer or Formulator

Type: manufacturer
Name of Plant: Houston Plant
Street: 1900 Tidal Road
Town: 77536 Deer Park, TX
Country: United States
Phone: 1-281-228-8100

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.0.3 Identity of Recipients

-

1.0.4 Details on Category/Template

-

1.1.0 Substance Identification

Smiles Code: CC(C)(CC(C)(N)C)C
Mol. Formula: C8H19N
Mol. Weight: 129.24

Source: Rohm and Haas Company, Sprign House, PA, USA
Reliability: (1) valid without restriction
17-MAY-2006

17-MAY-2006

1.1.1 General Substance Information

Purity type: typical for marketed substance
Substance type: organic
Physical status: liquid
Purity: ca. 97 - 100 % v/v
Colour: Clear, colorless liquid
Odour: Ammonia Odor

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.1.2 Spectra

-

1.2 Synonyms and Tradenames

Primene (TM) is a trademark of Rohm and Haas Company or one of its subsidiaries or affiliates.

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

Primene (TM) TOA Amine

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.3 Impurities

Purity type: typical for marketed substance

Remark: Contains small percentages of multiple side reactants.
Source: Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

Purity type: typical for marketed substance
CAS-No: 7732-18-5
EC-No: 231-791-2
EINECS-Name: water
Mol. Formula: H2O
Contents: = .2 - % v/v

Source: Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

1.4 Additives

Remark: Not applicable
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (1) valid without restriction
14-JUN-2006

1.5 Total Quantity

Quantity: > 700 tonnes produced in 2005

Source: Rohm and Haas Company, Spring House, PA, USA
22-JUN-2006

1.6.1 Labelling

Labelling: as in Directive 67/548/EEC
Symbols: (C) corrosive
(Xn) harmful
R-Phrases: (10) Flammable
(22) Harmful if swallowed
(34) Causes burns
S-Phrases: (26) In case of contact with eyes, rinse immediately with plenty of water and seek medical advice
(36/37/39) Wear suitable protective clothing, gloves and eye/face protection
(45) In case of accident or if you feel unwell, seek medical advice immediately (show the label where possible)

14-JUN-2006

1.6.2 Classification

Classified: as in Directive 67/548/EEC
Class of danger: harmful
R-Phrases: (10) Flammable
(22) Harmful if swallowed
(34) Causes burns

07-JUN-2006

1.6.3 Packaging

Memo: Packaged in either tank trucks, drums, pails, or small samples.

Source: Rohm and Hass Company, Spring House, PA, USA
07-JUN-2006

1.7 Use Pattern

Type: industrial
Category: other: Additive for petroleum products, corrosion inhibitor, rubber, coating resin, agricultural chemicals, pharmaceuticals, polyolefins, surfactants, heavy metal recovery

17-MAY-2006

1.7.1 Detailed Use Pattern

Industry category: 15/0 other
Use category: 55/0 other
Extra details on use category: No extra details necessary
No extra details necessary
Emission scenario document: not available

Remark: Fuel and lubricants, agricultural, pharmaceutcal, metals
17-MAY-2006

1.7.2 Methods of Manufacture

Type: Production

Remark: Test substance is manufactured in batch operations in kettles. All the product is hard-piped to temporary storage tank.
Source: Rohm and Haas Company, Spring House, PA, USA
05-JUL-2006

1.8 Regulatory Measures

-

1.8.1 Occupational Exposure Limit Values

Type of limit: other: Rohm and Haas Company
Limit value: 3 other: ppm
Short term exposure
Limit value: 9 other: ppm

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.8.2 Acceptable Residues Levels

-

1.8.3 Water Pollution

-

1.8.4 Major Accident Hazards

Legislation: other

Remark: Evacuate the spill area. Remove all sources of ignition. Floor may be slippery, use care to
avoid falling. Contain spills immediately with inert materials (e.g. sand, earth). Allow material to solidify and transfer solid material to separate suitable containers for recovery or disposal.
WARNING: KEEP SPILLS AND CLEANING RUNOFFS OUT OF MUNICIPAL SEWERS AND OPEN BODIES OF WATER.
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (1) valid without restriction
17-MAY-2006

1.8.5 Air Pollution

-

1.8.6 Listings e.g. Chemical Inventories

Type: EINECS
Additional Info: This product is also listed on the following countries product inventory:
Canada
China
Europe Union
Japan
Korea
Philippines

Source: Rohm and Haas Company, Spring House, PA, USA
14-JUN-2006

Type: TSCA

Source: Rohm and Haas Company, Spring House, PA, USA
14-JUN-2006

1.9.1 Degradation/Transformation Products

Type: degradation product

Remark: This material is considered stable under specified conditions of storage, shipment and/or use. There are no known hazardous decomposition products for this material. Product will not undergo polymerization.
17-MAY-2006

1.9.2 Components

-

1.10 Source of Exposure

Source of exposure: Human: exposure by production
Exposure to the: Substance

Remark: Eyes: Material can cause the following: corrosion to eyes; may cause permanent eye injury.
Skin: Material can cause the following: corrosion to the skin.
Ingestion: Harmful if swallowed.
Inhalation: Inhalation of vapor or mist can cause the following: irritation of the nose, throat and lungs, nausea, vomiting, pulmonary edema.

Source: Rohm and Haas Company, Spring House, PA, USA
17-MAY-2006

1.11 Additional Remarks

-

1.12 Last Literature Search

-

1.13 Reviews

-

2.1 Melting Point

-

2.2 Boiling Point

-

2.3 Density

Type: density
Value: = .7698 g/cm³

Method: other
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Method: Value was measured with the Anton-Paar DMA-46 densitometer. Samples were measured in duplicate.
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
Flag: Critical study for SIDS endpoint
17-MAY-2006

(9)

2.3.1 Granulometry

-

2.4 Vapour Pressure

-

2.5 Partition Coefficient

Partition Coeff.: octanol-water
log Pow: ca. 1.09

Method: other (measured)
GLP: no

Method: Shake Flask Method
Result: 1.09 +/- 0.20
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
17-MAY-2006

(7)

2.6.1 Solubility in different media

-

2.6.2 Surface Tension

Test type: other
Value: = 28 mN/m

Method: other
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Method: Value was measured on the Fisher Surface Tensiometer, Model 20. Two measurements were performed and the value is an average. The instrument was calibrated using hexane. The values obtained were within 2 dynes/cm from theoretical as given in the CRC handbook.
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
Flag: Critical study for SIDS endpoint
22-MAY-2006 (9)

2.7 Flash Point

Value: = 15.6 degree C
Type: closed cup

Method: other
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Method: Value was measured using Pensky-Martens closed cup.
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (2) valid with restrictions
No data on whether test was conducted in compliance with GLP, but test was conducted by recognized scientific standards.
Flag: Critical study for SIDS endpoint
17-MAY-2006 (9)

2.8 Auto Flammability

-

2.9 Flammability

-

2.10 Explosive Properties

-

2.11 Oxidizing Properties

-

2.12 Dissociation Constant

Method: other
GLP: no data
Test substance: as prescribed by 1.1 - 1.4

Method: Potentiometric titration in non-aqueous solvent was used. Using 75/25 isopropanol/octane solvent with 0.1N HCl in isopropanol as titrant, the Half Neutralization Potential (HNP) was determined. The HNP is the potential that develops when equimolar concentrations of nonionized acid and its derived ionized species are present. From this, the pKa value was estimated.

The titrator used was a Radiometer Titralab, equipped with a VIT90 Mark I controller, a SAM90 sample station and an ABU93 buret station. A standard glass electrode and a LiCl reference electrode were used for the titrations.

Remark: Due to poor solubility, titration directly in water to determine pKa value was not possible. Value was estimated from HNP.
Result: 10.5
Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (2) valid with restrictions
Flag: Critical study for SIDS endpoint
22-MAY-2006 (4)

2.13 Viscosity

-

2.14 Additional Remarks

Memo: Pour Point

Method: ASTM D-97
Result: Fluid at -65C
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: As prescribed by 1.1-1.4
Reliability: (2) valid with restrictions
17-MAY-2006 (9)

17-MAY-2006

3.1.1 Photodegradation

Type: other: AOPWIN estimation of hydroxyl radical reaction

Method: other (calculated)
GLP: no
Test substance: other TS

Method: AOPWIN v1.91
Remark: For hydroxyl radical reactions AOPWIN estimated the hydrogen abstraction rate constant to be 2.25E-12 cm3/molecule-sec. The reaction rate with N, S, and -OH was estimated to be 21.0E-12 cm3/molecule-sec. The overall OH radical rate constant was estimated to be 23.25E-12 cm3/molecule-sec. The estimated half-life equaled 5.52 hours assuming a 12 hour day and 1.5E06 OH/cm3. The model was unable to estimate ozone reaction kinetics because no structurally similar molecules were within the database.
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C(N)C)C
Reliability: (2) valid with restrictions
Value(s) derived using accepted calculation method/software.
22-MAY-2006 (5)

3.1.2 Stability in Water

Method: other (calculated)
GLP: no
Test substance: other TS

Method: HYDROWIN v1.67
Remark: HYDROWIN was unable to estimate hydrolysis rate constant because no similar chemical structures are in the database.
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C)(N)C)C
Reliability: (2) valid with restrictions
Value(s) derived using accepted calculation method/software.
22-MAY-2006 (5)

3.1.3 Stability in Soil

-

3.2.1 Monitoring Data (Environment)

-

3.2.2 Field Studies

-

3.3.1 Transport between Environmental Compartments

Type: other: Fugacity Model Level I and III
Media: other: air, water, soil, sediment
Method: other
Air: 66.1 % **(Fugacity Model Level I)**
Water: 25.3 % **(Fugacity Model Level I)**
Soil: 8.5 % **(Fugacity Model Level I)**
Biota: 79.1 % **(Fugacity Model Level II/III)**
Soil: .0004 % **(Fugacity Model Level II/III)**

Remark: Default values were assumed for environmental compartment descriptions, dimensions, and advective and dispersive properties.
Chemical-specific physical properties (at 25 deg. C) used as model input parameters were:

Molecular weight: 129.25
Water Solubility: 10670 (mg/L)
Vapor pressure: 8.03 mm Hg, 1070.58 Pa (estimated using MPBPWIN)
Log Kow: 2.58 (estimated using KOWWIN)
Melting Point: -20.02 (estimated using MPBPWIN)
Half-lives (h):
Air: 11
Water: 900
Soil: 1.8E03
Sediment: 8.1E03
Half-lives were calculated by the model based on the properties of the test substance.

Result: Level I

Compartment	Mass (percent)	Half-life (hr)
Air	66.1	11
Water	25.3	900
Soil	8.50	1.8E03
Sediment	0.189	8.1E03

Level III

Compartment	Mass (percent)
Air	1.02
Water	19.7
Water: Fish	3.74E-04
Soil	79.1
Sediment	0.187

Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine [CAS No. 107-45-9]; SMILES: CC(C)(CC(C)(N)C)C
Reliability: (2) valid with restrictions
Value(s) derived using accepted calculation method/software.

22-MAY-2006 (5)

3.3.2 Distribution

-

3.4 Mode of Degradation in Actual Use

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3.5 Biodegradation

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3.6 BOD5, COD or BOD5/COD Ratio

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3.7 Bioaccumulation

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3.8 Additional Remarks

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AQUATIC ORGANISMS

4.1 Acute/Prolonged Toxicity to Fish
-

4.2 Acute Toxicity to Aquatic Invertebrates
-

4.3 Toxicity to Aquatic Plants e.g. Algae
-

4.4 Toxicity to Microorganisms e.g. Bacteria
-

4.5 Chronic Toxicity to Aquatic Organisms

4.5.1 Chronic Toxicity to Fish
-

4.5.2 Chronic Toxicity to Aquatic Invertebrates
-

TERRESTRIAL ORGANISMS

4.6.1 Toxicity to Sediment Dwelling Organisms
-

4.6.2 Toxicity to Terrestrial Plants
-

4.6.3 Toxicity to Soil Dwelling Organisms
-

4.6.4 Toxicity to other Non-Mamm. Terrestrial Species
-

4.7 Biological Effects Monitoring
-

4.8 Biotransformation and Kinetics
-

4.9 Additional Remarks

-

5.0 Toxicokinetics, Metabolism and Distribution

-

5.1 Acute Toxicity

5.1.1 Acute Oral Toxicity

Type:	LD50
Species:	rat
Strain:	other: Crl:CD BR
Sex:	male/female
No. of Animals:	12
Vehicle:	other: none
Doses:	50, 150, 200, 500 and 2000 mg/kg bw
Value:	= 217.7 mg/kg bw
Method:	OECD Guide-line 401 "Acute Oral Toxicity"
Year:	1991
GLP:	yes
Test substance:	as prescribed by 1.1 - 1.4

Method:

Groups of 12 rats (6/sex) were quarantined for approximately one week, then administered the test substance at dose levels of 50, 150, 200, 500 and 2000 mg/kg. The initial body weight ranges reported were 186 to 215 g for males and 186 to 214 g for females.

The test substance was delivered orally as a single gavage dose undiluted. Rats were fasted overnight prior to dosing. All rats had free access to filtered tap water and feed (Purina Certified Rodent Chow). Animals were housed 2 or 3 per cage and maintained at a temperature of 24oC and a relative humidity range of 40 to 65%. All animals were observed for signs of ill health, or reaction to treatment at 1, 2 and 4 hr after dosing and once daily thereafter for 14 days, and were necropsied following death, as it occurred, or at the end of the observation period.

Result:

LD50 values were calculated from the logarithm of the doses and the incidences of mortality using a SAS PROBIT procedure based on the method of D.J. Finney (1971).

Mortality (number of dead /number of animals tested): Dose 50, 150, 200, 500, 2000 mg/kg; Males 1/6, 2/6, 2/6, 6/6, 6/6, respectively; Females 1/6, 0/6, 3/6, 4/5, 6/6, respectively; Combined 2/12, 2/12, 5/12, 10/11, 12/12, respectively.

The LD50 was calculated on the combined mortality incidence data. The acute oral LD50 in male and female rats (combined) was 217.7 mg/kg, with 95% confidence limits of 142.9 and 352.3 mg/kg.

Numerous clinical signs were observed in all doses. These signs included, but were not limited to, ataxia, circling, disoriented behavior, gasping, lacrimation, passiveness, ptosis, tremors and wheezing. Signs found in decedents only were abdominal breathing, arched back, cage biting, emaciation, labored breathing, lethargy and prostration.

Necropsy of decedents revealed the following gross changes related to test substance: black foci on stomach mucosa, clear fluid, mucous-like material and black material (viscera autolyzed) in stomach, distention of intestines and stomach, intestines (including cecum) filled with air, matted fur on muzzle, mucous material in stomach, tan and red staining of the muzzle, red stained eyes, reddened lungs, intestines and cecum, severe reddening of the stomach, tan and/or yellow-stained anogenital area. However, necropsy of the survivors revealed no gross changes related to the test substance.

Source: Rohm and Haas Company, Spring House, PA, USA
Reliability: (1) valid without restriction
Flag: Critical study for SIDS endpoint
02-AUG-2006 (1)

Type: other
Species: rat

GLP: no
Test substance: other TS

Result: Toxic
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006 (6)

5.1.2 Acute Inhalation Toxicity

Type: other
Species: rat

GLP: no
Test substance: other TS

Result: Toxic

All rats dead within 15 minutes.
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006 (6)

5.1.3 Acute Dermal Toxicity

Type: other
Species: rabbit

GLP: no
Test substance: other TS

Result: Essentially non-toxic
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006

(6)

5.1.4 Acute Toxicity, other Routes

-

5.2 Corrosiveness and Irritation

5.2.1 Skin Irritation

Species: rabbit
Exposure: Occlusive
Exposure Time: 4 hour(s)
No. of Animals: 6
Vehicle: other: none
Result: corrosive

Method: OECD Guide-line 404 "Acute Dermal Irritation/Corrosion"
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Method: Occlusive patch test. 0.5 mL applied topically to the shaved intact skin of six New Zealand White rabbits. The application sites were occluded for 4 hours. Skin irritation was evaluated according to the Draize criteria at approximately 1, 24, 48 and 72 hours and 7 and 14 days after patch removal.

Result: No mortality or clinical signs were observed. Severe erythema and severe edema were observed at 1 hour. Edema was no longer evident by 72 hours; however, severe erythema continued through to day 14 of the study. Beginning at 24 hours, eschar or concave eschar was observed. On day 14, concave eschar, peripheral scar formation and deep narcosis were observed. The 72 hour Mean Irritation Score (MIS) was 4.0. On day 14, it was concluded that there was irreversible destruction of dermal tissue.

Source: Rohm and Haas Company, Spring House, PA, USa
Reliability: (1) valid without restriction
22-MAY-2006

(3)

GLP: no
Test substance: other TS

Result: Score 4.7
Not a primary skin irritant, however, test material would be considered a moderate irritant.
Source: Rohm and Haas Company, SPring House, PA, USA
Test substance: t_octylamine, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006 (6)

5.2.2 Eye Irritation

Test substance: as prescribed by 1.1 - 1.4

Remark: Because t-Octylamine produced corrosive effects to the skin of rabbits, it was determined that the sample be categorized as corrosive to the eyes of rabbits.

Present animal testing guidelines indicate that (i) materials which have demonstrated definitive corrosion or severe irritation in a skin irritation study need not be further tested for eye irritation, and (ii) it may be presumed that substances will produce similarly severe effects in the eyes.
Source: Rohm and Haas Company, Spring House, PA, USA
22-MAY-2006 (2)

Species: rabbit

GLP: no
Test substance: other TS

Result: Essentially non-toxic
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylaime, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006 (6)

GLP: no
Test substance: other TS

Result: Marked eye irritant
Source: Rohm and Haas Company, Spring House, PA, USA
Test substance: t-Octylamine, clear liquid, purity not reported
Reliability: (4) not assignable
22-MAY-2006 (6)

5.3 Sensitization

-

5.4 Repeated Dose Toxicity

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5.5 Genetic Toxicity 'in Vitro'

Type: Ames test
System of testing: Salmonella typhimurium strains TA1535, TA1537, TA98, TA100
Concentration: 50, 200, 500, 2000 and 5000 ug/plate
Metabolic activation: with and without
Result: negative

Method: OECD Guide-line 471
Year: 1995
GLP: yes
Test substance: as prescribed by 1.1 - 1.4

Method: Strains of Salmonella typhimurium used for this study included: TA98, TA100, TA1535 and TA1537 obtained from Dr. B. Ames, University of California, Berkeley. Strains were characterized for nutritional requirements, crystal violet sensitivity and ampicillin resistance no more than 6 months prior to initiation of the study. The solvent for the test article and the positive control articles (with the exception of sodium azide and 9-aminoacridine) was dimethyl sulfoxide (DMSO). The solvent for sodium azide was distilled water. The solvent for 9-aminoacridine was 95% ethanol.

The positive control, in the presence of metabolic activation, was 2 ug/plate 2-anthramine, for all four strains. In the absence of metabolic activation, the positive controls were 3 ug/plate 2-nitrofluorene for strain TA98; 2 ug/plate sodium azide for strains TA100 and TA1535; and 100 ug/plate 9-aminoacridine for strain TA1537.

The S-9 used for metabolic activation was obtained from rats induced with Aroclor 1254.

The test article was evaluated for mutagenic activity at concentrations ranging from 50 to 5000 ug/plate, with and without metabolic activation, in Salmonella strains TA98, TA100, TA1535 and TA1537. Control plates were run to check for sterility, determine the background reversion rate, and measure the response of each tester strain to a positive control compound.

For the activated portion of the assay the following were added, in order, to sterile test tubes: 2 mL of top agar, 0.1 mL of the bacteria inoculum, 0.1 mL of the appropriate concentration of test compound, and 0.5 mL of phosphate buffer mix (with S-9 and NADP). For the non-activated portion of the assay, the above procedure was followed, except that

the 0.5 mL of phosphate buffer mix (without S-9 or NADP) was added to the tubes directly after addition of the top agar. Each test article concentration was tested in triplicate, in minimal plates (minimal-glucose agar medium). The controls were tested in six replicates in minimal plates. The contents of the tubes were mixed and poured onto petri dishes containing approximately 19 mL of the appropriate agar. Plates were allowed to set for several minutes then placed in covered plastic boxes and incubated at 37 (+ 1) degrees Celsius for approximately 72 hours prior to colony counting.

Following the incubation period, sterility plates were checked for contamination. Following the sterility check, the number of colonies on each plate was determined. The mean and standard deviation for each concentration was calculated. Background growth was checked for each experimental point to observe any toxic response.

A mutagenicity assay is considered valid if the following conditions are met. First, the spontaneous reversion rate, with and without metabolic activation, must be reasonably consistent with the expected range for the strain being used. Second, the positive control materials must elicit a positive response. And third, the strains must maintain characteristics.

A test article is considered positive if it elicits in independent assays a number of revertants per plate at least 2 times that observed in the solvent control (background). A response that does not meet this criteria but elicits a potential biologically significant is considered an equivocal response and requires further evaluation.

A test article is considered negative if the criteria for a positive assay were not met and the test article was tested up to either 5000 ug/plate, the limit of solubility, or the limit of toxicity. Toxicity is defined as the elimination of a uniform background lawn.

Result: The test article was evaluated at 50, 200, 500, 2000 and 5000 ug/plate in the presence and absence of S-9.

The study was designed to evaluate the mutagenic potential of the test article up to the limits of solubility, toxicity or 5000 ug/plate (whichever was lower). A contaminant was observed in TA98 and TA1537 in several plates at various dose levels. The contamination was minimal and did not interfere with scoring. A mutagenic response was not detected in any of the four tester strains (TA98, TA100, TA1535 and TA1537) in any of the experiments conducted.

Under the conditions of this study, the test substance was not mutagenic in the Salmonella gene mutation assay.

Source: Rohm and Haas Company, Spring House, PA, USA

Reliability: (1) valid without restriction

Flag: Critical study for SIDS endpoint
22-MAY-2006 (8)

22-MAY-2006

5.6 Genetic Toxicity 'in Vivo'

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5.7 Carcinogenicity

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5.8.1 Toxicity to Fertility

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5.8.2 Developmental Toxicity/Teratogenicity

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5.8.3 Toxicity to Reproduction, Other Studies

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5.9 Specific Investigations

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5.10 Exposure Experience

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5.11 Additional Remarks

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6.1 Analytical Methods

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6.2 Detection and Identification

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7.1 Function

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7.2 Effects on Organisms to be Controlled

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7.3 Organisms to be Protected

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7.4 User

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7.5 Resistance

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8.1 Methods Handling and Storing

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8.2 Fire Guidance

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8.3 Emergency Measures

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8.4 Possib. of Rendering Subst. Harmless

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8.5 Waste Management

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8.6 Side-effects Detection

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8.7 Substance Registered as Dangerous for Ground Water

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8.8 Reactivity Towards Container Material

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10.1 End Point Summary

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10.2 Hazard Summary

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10.3 Risk Assessment

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